

## **5. THREE DIMENSIONAL MODELLING OF THE BIOPOLYMER STRUCTURE OF THE PLANT CELL WALL II.**

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### **Abstract**

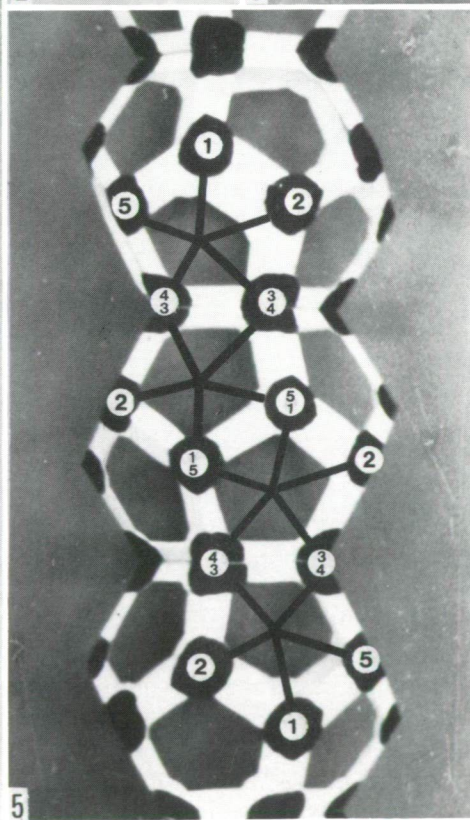
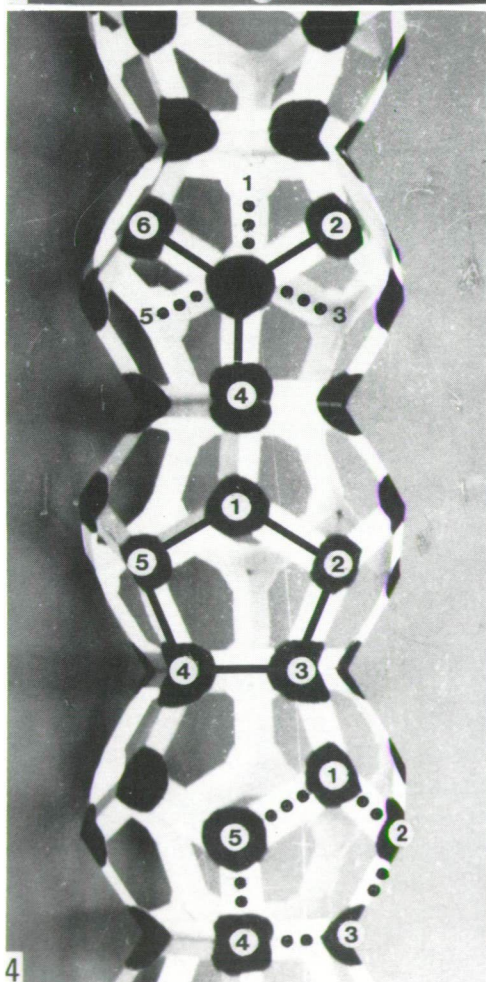
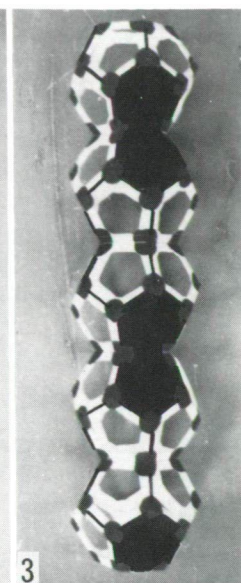
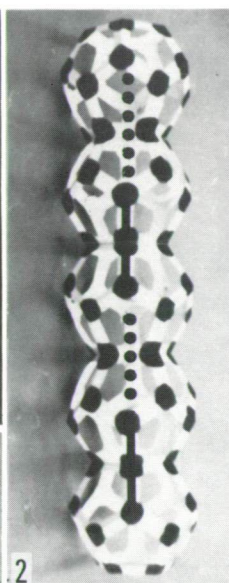
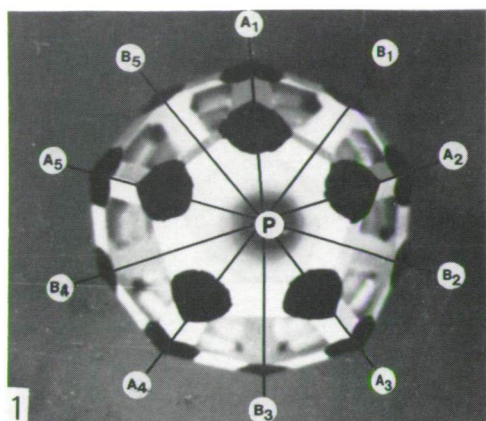
On the basis of the elementary (basic) units of the structural highly organized biopolymer skeleton the following types were distinguished: 1. Primary units; filaments, lamellae, helical, microtubular, globular (PENROSE-like) highly organized biopolymer skeleton structural elements. The basic (building) unit is a pentagonal dodecahedron elementary unit. 2. Secondary units; filaments and the further above mentioned elements of the plant cell wall and the cytoskeleton, but composed from PENROSE-I type biopolymer skeleton. In this way the building unit is composed of 13 pentagonal dodecahedron elementary (basic) units. This paper summarizes the results of the modelling as follows. 1. Filaments including the primary and the secondary biopolymer skeleton. 2. PENROSE-I and PENROSE-II units. 3. Helical (microtubular) secondary unit. 4. Primary modelling of the lamellar system. 5. Particular attempt was bestowed upon the biopolymer skeleton of the surface. It was established that quasi-periodic units in linear or two dimensional systems can be periodic, too.

*Key words:* Plant cell, biopolymer organization, three-dimensional modelling.

### **Introduction**

As it was emphasized in the previous paper (KEDVES, 1991b) the three-dimensional modelling of the quasi-crystalloid biopolymer skeleton will be continued. The first models presented, and discussed in the above mentioned paper were prepared following the most important problems which arose in our last two-dimensional modelling (KEDVES, 1991a; KEDVES and FARKAS, 1991), and the new TEM data concerning the partially degraded plant cell walls. It is clear that our knowledge about the three-dimensional structure of the quasi-crystalloid biopolymer skeleton can not be taken as completely accomplished. But we hope that now we have enough data to have notions concerning this complicated biopolymer system of the most important cellular elements. Besides the highly organized biopolymer structures, particular attention was paid for the surface and/or for the bordering layers of the cellular organelles.

On the basis of our up-to-date knowledge about the quasi-crystalloid skeleton of the plant cell wall, and of the newest experimental results we have the



opportunity to start the combined modelling, which contains two important fields:

- i. Investigation of the detailed quasi-crystalloid skeleton.
- ii. The modelling of the stabilizing biopolymer system. This latter is also heterogeneous in character. The detailed study of the stabilizing molecular system including its modelling will be the subject of further investigations.

◀ Plate 5.1.

1—5. Quasi-crystalloid skeleton model of the primary filament.

1. Aspect of the quasi-crystalloid skeleton model. In this view the picture is similar to one pentagonal dodecahedrane model. "P" is in the axe of the filament.  $AP_{1-5}$  and  $BP_{1-5}$  are the axes of the primary rotations.
- 2,3. Two aspect of first importance of the primary filament.
2. Periodic lateral short axis view. The so-called proximal and distal short axes are in the same plane.
3. Discontinous short axis view. Short axes alternate with two planes of the dodecahedrane.
- 4,5. Details from the above mentioned two aspects of first importance of the model of the primary filament.
4. The important points of symmetries, or biopolymer units (globular) of the model are indicated. The two times three-fold symmetry can be pointed out.
5. Five-fold points of symmetries of the alternating pentagonal planes.

## Methods

The basic — building elementary — units are as it was published in the previous part of this series of papers. Some minor alterations were introduced only as follows.

- i. The central biopolymer unit of the PENROSE-I model is no more compact. It is identical with the basic pentagon dodecahedrane unit.
- ii. Some alterations were introduced in the colouring of the modelling units to better understand the characteristic features of the biopolymer skeleton, and its points of symmetries in the space.

## Results

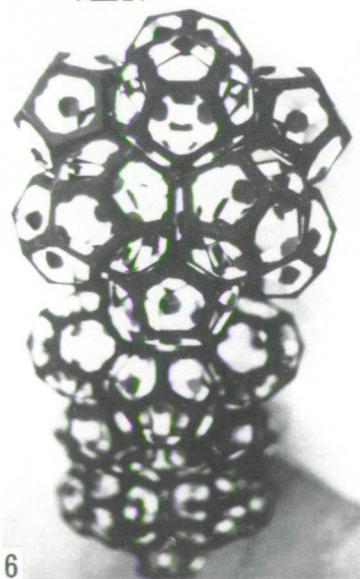
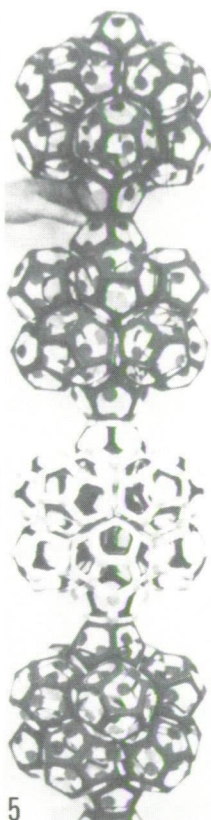
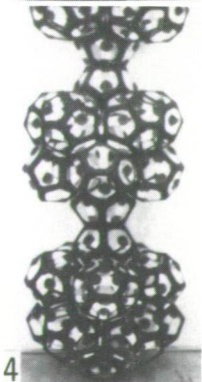
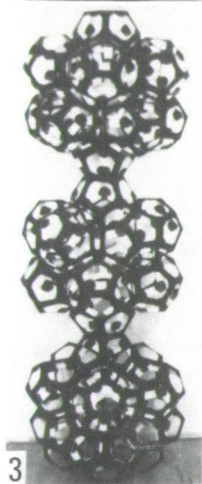
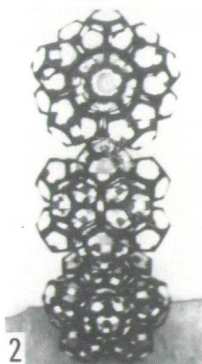
### FILAMENTS

#### Primary (simple) filaments (Plate 5.1., figs. 1—5)

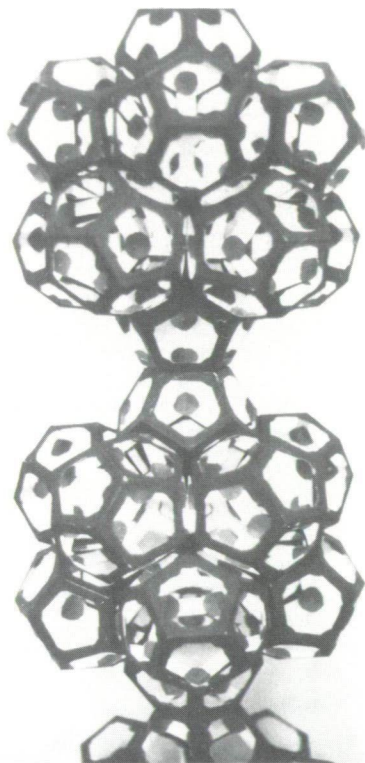
The most important characteristic features of this kind of highly organized biopolymer unit are as follows.

The linear arranged dodecahedron basic skeleton units are connected by five edges, or better to say with one plane of each dodecahedron. In this way there are no frustrations between the building units of this kind of biopolymer skeleton, and it is a peculiar periodical arrangement. At this kind of periodical system two dodecahedron basic skeleton represents one unit (Plate 5.1., fig. 2,3, resp. 4,5).

The three-dimensional quasi-crystalloid units arranged in one linear system accomplish a periodic skeleton.



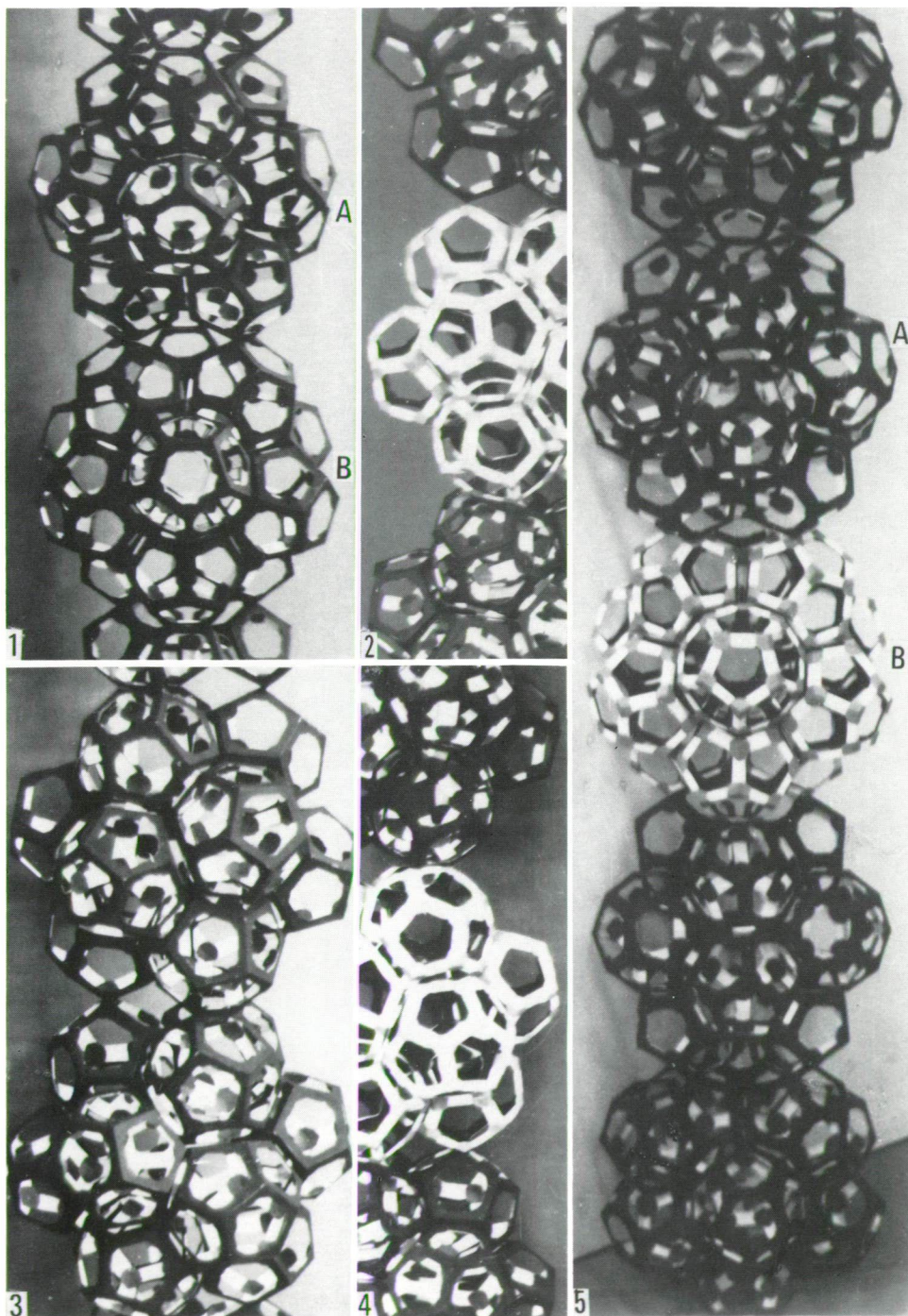
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◀ Plate 5.2.

- 1—8. First type of connections of the secondary (complex) filament.
1. Aspect of the quasi-crystalloid skeleton model of the first type of connecting the secondary filament. In this view the picture of this kind of model of quasi-crystalloid filament is similar to one PENROSE—I quasi-crystalloid unit. The regular pentagon in the middle is identical in the point of view of the rotation axes with those illustrated in Plate 5.1., fig. 1.
- 2—4. Homogeneous complex filament from different views. The elementary PENROSE—I units from these views can be pentagonal or hexagonal.
5. Lateral view of the model of a heterogeneous filament.
6. Oblique lateral view of a homogeneous secondary filament. It is noteworthy that the connections between the PENROSE—I building units are discernible.
- 7, 8. Magnified pictures from the connecting units of a homogeneous secondary filament from somewhat different lateral views. The alternation of the position of the points of symmetries is interesting and important.





The aspect of the filament (Plate 5.1., fig. 1) well illustrates essentially the symmetries of the quasi-crystalloid basic units (cf. Plate 7.1., fig. 1, KEDVES 1991b, p. 68). In the pictures taken from the lateral views of the model of the filaments the above mentioned periodic characteristic features can be well studied. It seems that there are a lot of opportunities for the investigation of the aspects, two most important views are represented as follows.

1. Periodic lateral short axis view (Plate 5.1., fig. 2,4)

The plane of the short axes is identical with the plane crossing the  $B_5-P-A_1$  line. The different views well represent the different aspects of the pentagonal units. But two times three-fold points of symmetries can also be occur in consequence of the particular superposition of the edges of the pentagon dodecahedrane unit (Plate 5.1., fig. 4).

2. Short axes with planes alternate views (Plate 5.1., fig. 3,5)

In contrast to the previous aspect it is not an axis view. Fig. 3 in Plate 5.1., illustrates well that the short axes end at the apices of a peculiar octahedron composed of two sides of two connected pentagon dodecahedrane units. Fig. 5, of Plate 5.1., illustrates well the connecting globular units, and the AP axes of one unit composed of four pentagons. It is clearly shown that there are differences in the two middle planes in contrast to the first and the fourth pentagon. In this case, the essential differences came from the 5—5 connecting globular units of two pentagonal sides. This plane represents the first circle of points of symmetries composed of 5 points, cf.  $A_1, A_2, A_3, A_4$  and  $A_5$  of fig. 1, Plate 10.1. The lateral zigzag, in the view of the filament represents the second circle, composed of 10 points of symmetries of the edges, cf.  $A_1, B_1, A_2, B_2, A_3, B_3, A_4, B_4, A_5, B_5, A_6, B_6, A_7, B_7, A_8, B_8, A_9, B_9, A_{10},$  and  $B_{10}$  of fig. 1, Plate 5.1.

### Secondary (complex) filaments (Plate 5.2., figs. 1—8., plate 5.3., figs. 1—5)

In this case the building elements are the PENROSE-I units. Based on our up-to-date knowledge four secondary filament types have been distinguished, on the basis of two points of views, as follows.

- i. The building PENROSE-I units may be homogeneous or heterogeneous.

#### ◀ Plate 5.3.

1—5. Second type of connecting the secondary (complex) filament.

1, 3. Homogeneous complex filament from two important views.

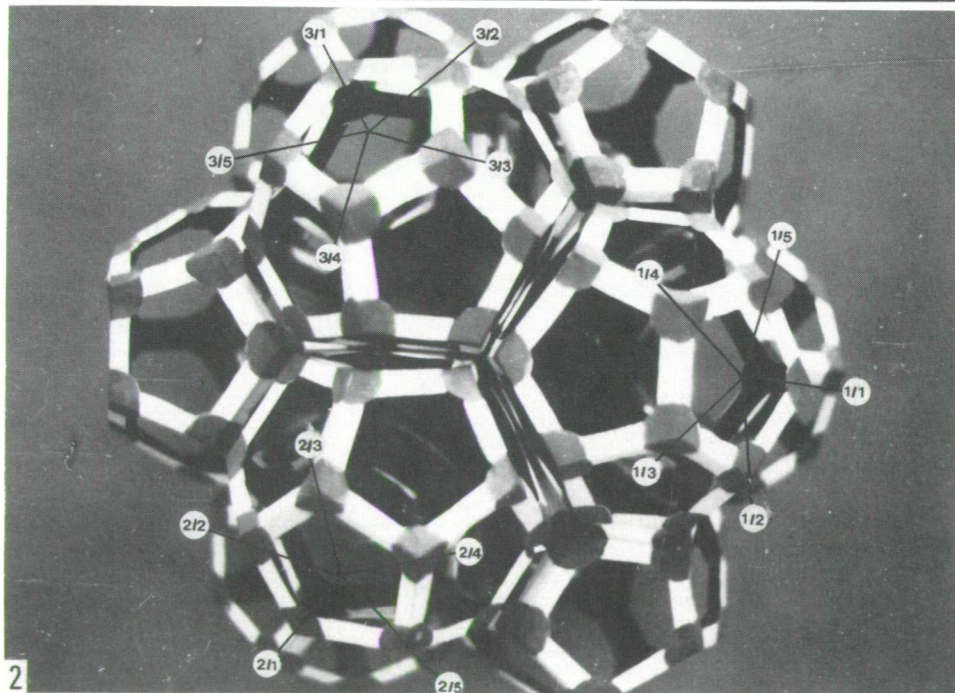
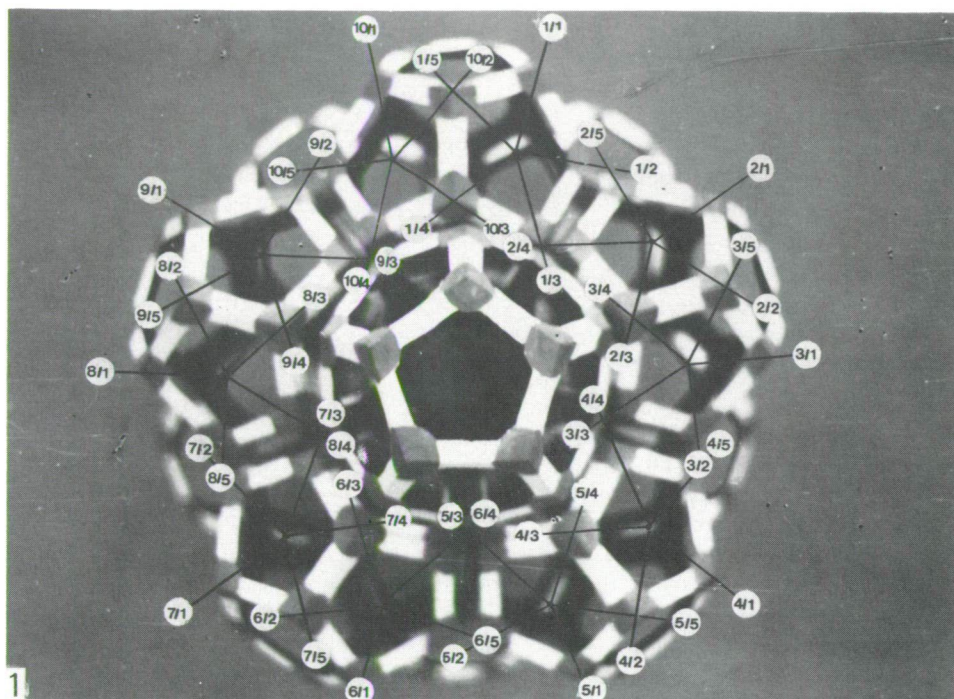
1. The building PENROSE—I units are in two kinds of symmetry position; A=The contour is hexagonal, in the centre a triangular symmetry is characteristic. B=Pentagonal contour in the centre with basic regular pentagonal polygon.

3. The lateral view; the connecting apices are in the middle of the filament.

2,4. Detail from the lateral part of the heterogeneous complex filament.

5. General aspect of the heterogeneous complex filament. This view corresponds to those represented in fig. 1, is perpendicular to the middle point of one connecting side.







Concerning this problem it is necessary to emphasize that at this kind of filaments, at this moment it is hypothetical that different kinds of molecular structures can occur in the same quasi-crystalloid biopolymer skeleton system (Plate 5.2., fig. 5., plate 5.3., fig. 2, 4, 5).

ii. Following the connecting points of symmetries, further two major types can be distinguished:

Five points of symmetries, respectively one plane of each PENROSE-I unit (Plate 5.2., figs. 1—8) are connected. In this case the axe of this secondary filament is essentially identical with those of the primary (simple) filament with the above mentioned periodicity. Each PENROSE-I unit contributes with three basic pentagon dodecahedrae. These are in the axis of this unit. The alternation of the PENROSE-I unit is identical with the two principal aspects of the PENROSE-I model, illustrated in the 5.4., fig. 1,2.

The second connection type is the so-called PENROSE-II. In this case three times one side, or two times six points of symmetries are connected. In the previous paper the frustration between 8 points of symmetries (or globular biopolymer units) was emphasized (KEDVES 1991b, p. 70, fig. 1).

The axe of this kind of filament is in the middle of three pentagonal polygon sides. This characteristic feature completely differs from the above mentioned ones. The previously established axes which across the centrum of two opposite pentagonal polygon units is a form of zigzag. The angles of these axis parts are  $60^\circ$ . It is an interesting alternate periodicity, in this case there are PENROSE-I type units, having such axis too, which are completely at the right angles to the composite filament axis (B). It is self understanding, that there are a lot of further axes.

## DIFFERENT ORGANIZATION LEVELS OF THE PENROSE-UNITS

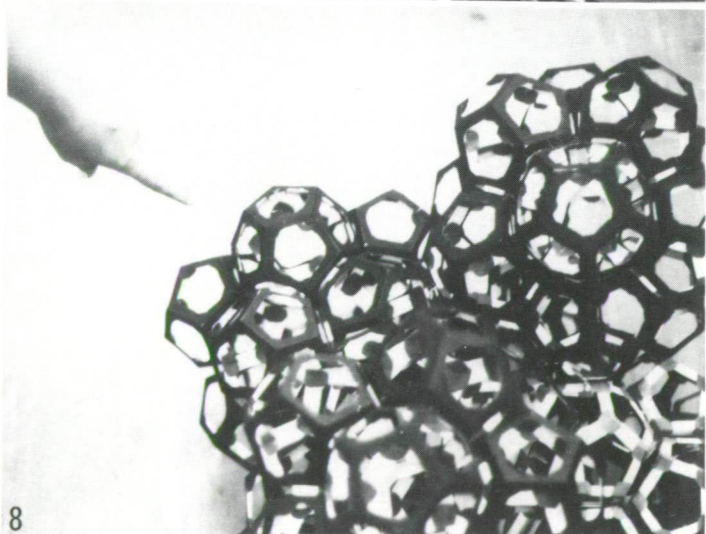
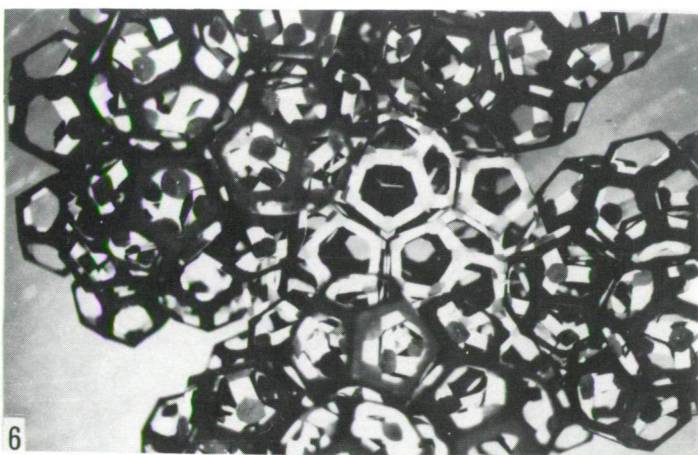
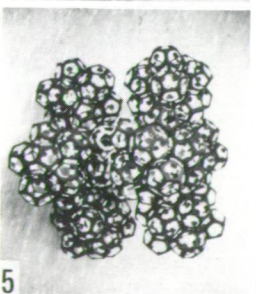
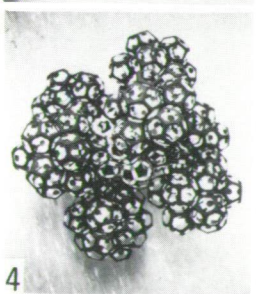
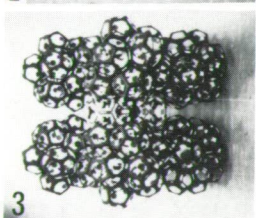
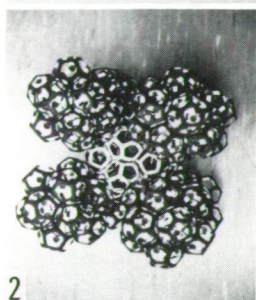
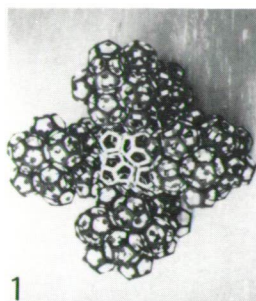
### Penrose-I type biopolymer skeleton (Plate 5.4., fig. 1,2)

As it was emphasized previously, this kind of biopolymer model was prepared and discussed in the first part of this series of papers, but in a little different manner, the central pentagon dodecahedron was compact. Moreover an attempt was made to start the investigation of the PENROSE-II quasi-crystalloid model (cf. KEDVES 1991b, Plate 7.2., fig. 1,2, p. 70).

This unit is extremely important in the further organization levels of the biopolymer skeleton, as the “basic unit”. This was pointed out previously, too, in

#### ◀ Plate 5.4.

- 1,2. Two major views in the symmetry of the PENROSE—I quasi-crystalloid biopolymer skeleton.
1. Quasi-periodic view of the PENROSE—I skeleton. The contour is pentagonal. The primary rotation axes are indicated on the outer (“second circle”) of pentagonal polygons.
2. The PENROSE—II connection view of the same PENROSE—I model. The contour is hexagonal, and no central regular pentagon is in the centre.



◀ Plate 5.5.

- 1—8. Modelling of the PENROSE—II biopolymer skeleton.
- 1—7. First step of the modelling of the PENROSE—II biopolymer skeleton. The light, central PENROSE—I skeleton is surrounded with eight further, “surrounding PENROSE—I” units. The connection between these PENROSE—I units is the so-called classical PENROSE—II connection; two times three sides (12 edges, or globular biopolymer units of the pentagons).
- 1—5. The first step in the building of the PENROSE—II biopolymer skeleton model from different aspects.
- 6,7. Detail from the central and the surrounding PENROSE—I biopolymer units. The great number of points of symmetries is noteworthy.
8. One PENROSE—I biopolymer unit, connected with the second step type connection. At this kind of connection the surrounding PENROSE—I skeleton does not reach the central PENROSE—I biopolymer unit. The connections are with the “first step connected” surrounding biopolymer units. The left hand of Mrs. BIRÓ—HALÁSZ indicates this unit.

connection with the organization systems of the filaments, it is necessary to add some methodical establishments, as follows.

i. There are two major views in the symmetries (Plate 5.4., fig. 1,2)

At the first one, the view axis is at the right angle to the plane of one pentagonal side. In this way, the concentric points of symmetries are well shown. The probable rotation axes are indicated at the “second circle” of pentagons. As it was very characteristic at the quasi-crystalloid skeleton of the filaments, the AP axis is a constant line.

It is important that the contour of the PENROSE—I unit from this view is a regular pentagon, in this way essentially this is a quasi-periodic system.

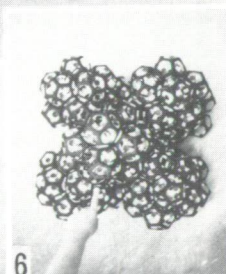
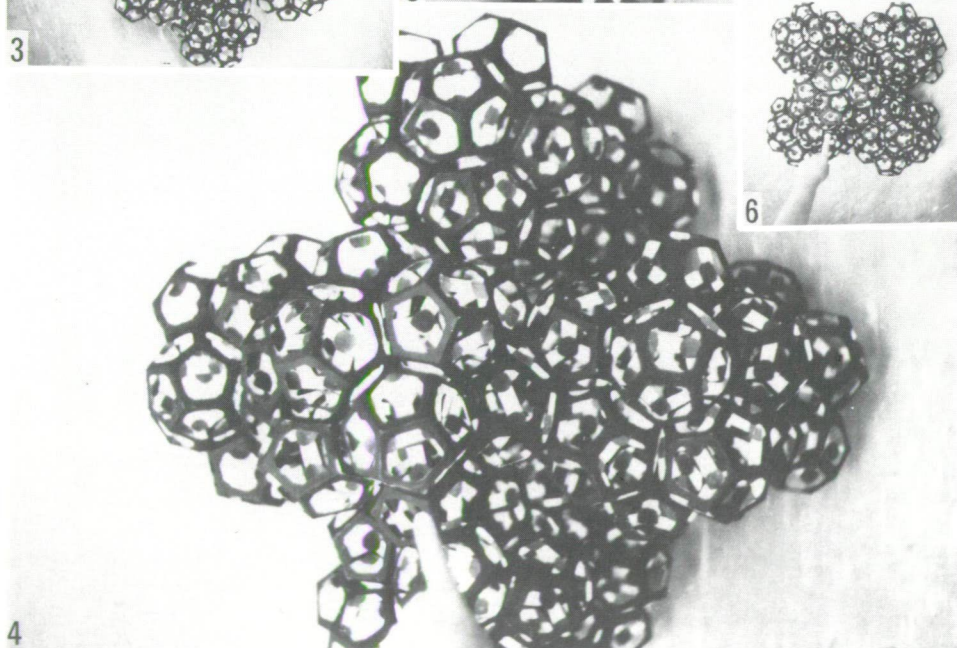
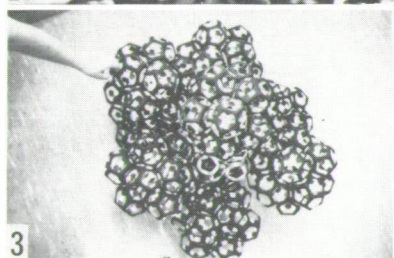
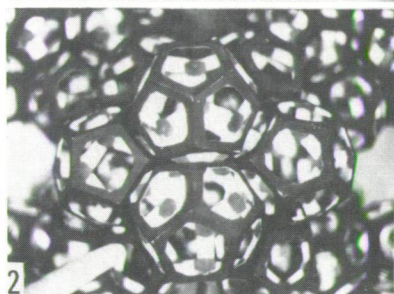
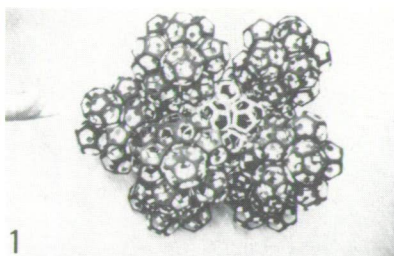
ii. The same model in the so-called PENROSE—II connection view (six points, or three sides) have a hexagonal contour, so this seems to be a periodic unit. No central pentagon, the axis of this unit is the middle points of three apices of pentagonal sides. The rotation axes of three pentagonal polygon sides are indicated. This is also for the better understanding and interpretation of our TEM pictures of the partially degraded plant cell walls, and the results of its rotations.

Penrose—II biopolymer unit  
(Plate 5.5., figs. 1—8, plate 5.6., figs. 1—6)

To better understand this complicated model the coloration of the central PENROSE—I skeleton was prepared in a different manner; the lighter skeleton. After starting the building of the complete “big PENROSE—II” biopolymer skeleton model we observed as follows.

Eight „surrounding PENROSE—I” units can be connected to the central unit, with the so-called classical connection, two times three sides (12 edges, or globular biopolymer units of the pentagons). From different views this, not complete PENROSE—II biopolymer skeleton have tetragonal, pentagonal, or hexagonal ambitus. The diameter of the “tetragonal view” is about 144 Å, the maximum size of the hexagonal one is 154 Å (Plate 5.5., figs. 1—5). Fig. 6 and 7 illustrate well the really complicated points of symmetry system around the central PENROSE—I skeleton from different views, and the large holes between the “surrounding” or “satellite” PENROSE—I system.





◀ Plate 5.6.

- 1—6. The first step connected PENROSE—II biopolymer model with one second type connected PENROSE—I unit. The pictures were taken from different positions and magnifications. The “second step connected” PENROSE—I unit is indicated by Mrs. BIRÓ—HALÁSZ. It is noteworthy that without indication it is almost impossible to observe the differences between the two kind connected surrounding PENROSE—I units.

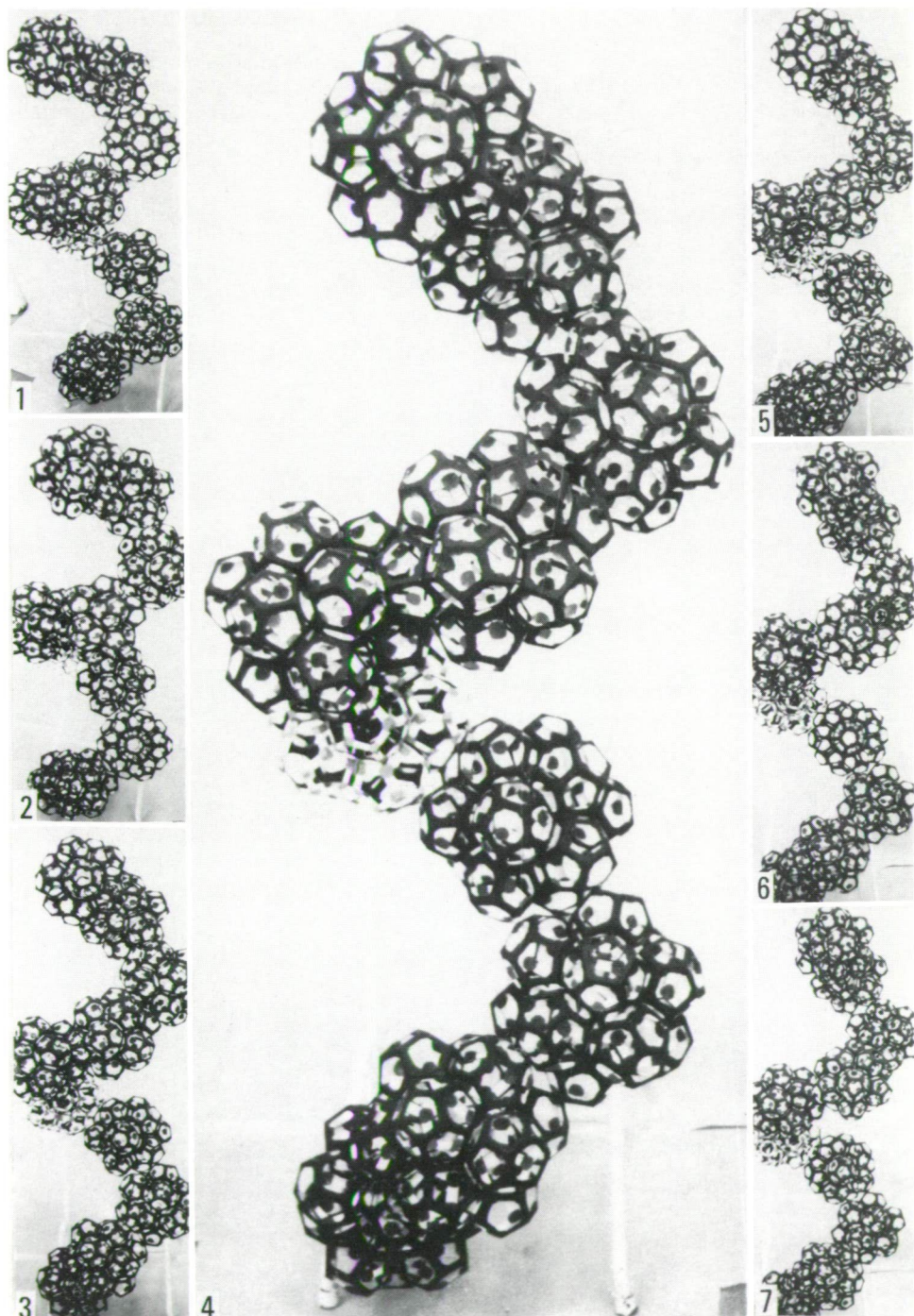


Plate 5.7.

1—7. Heterogeneous secondary helical biopolymer skeleton. The pictures were taken from different positions and magnifications from the same model.



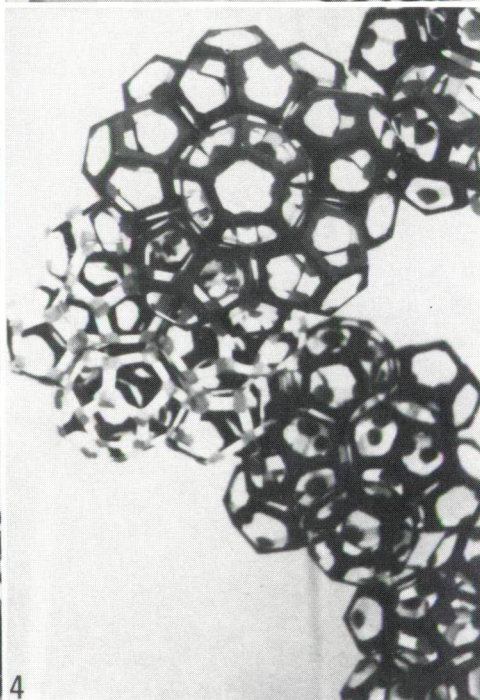
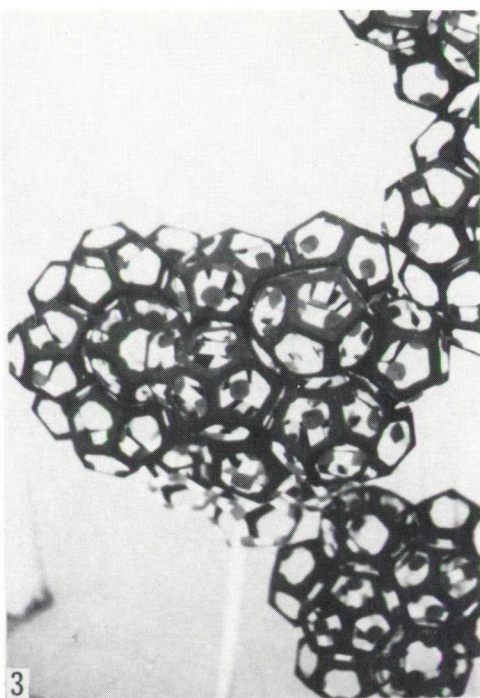
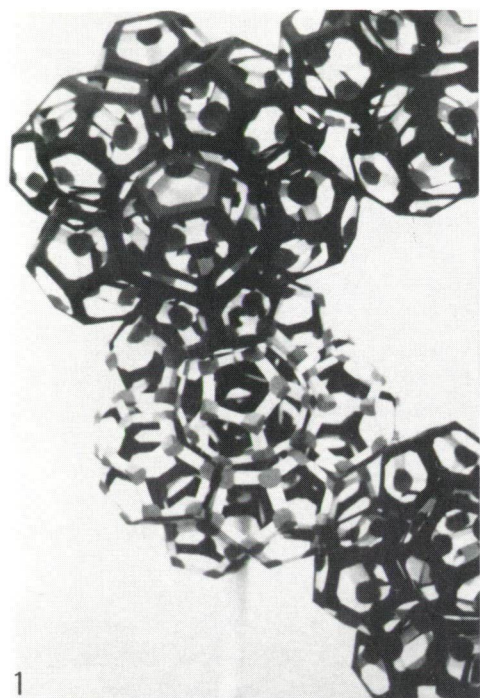
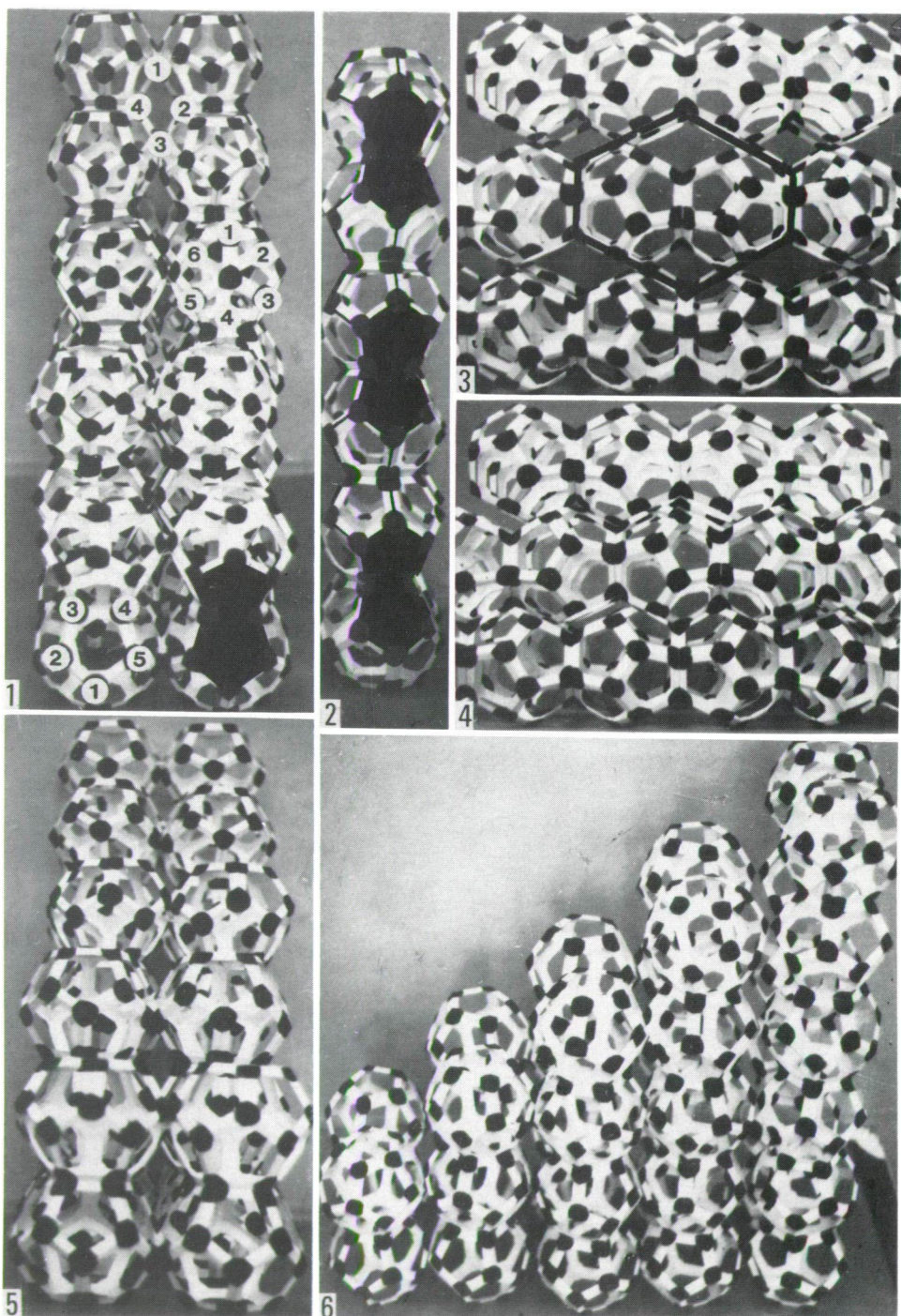


Plate 5.8.

1—4. Details from the connections and points of symmetries of the secondary helical biopolymer model.





To complete the large PENROSE—II skeleton we have not enough model but we started this. One PENROSE—I unit was connected to this system, in a completely different manner. Fig. 8 in Plate 5.5. and figs. 1—6 of Plate 5.6. illustrate well this skeleton. The hand of Mrs. BIRÓ—HALÁSZ indicate this ninth PENROSE—I unit, which may be said as the first of the second type of connections in the complete PENROSE—II biopolymer skeleton system. On the basis of our up-to-date knowledge the most important characteristic features of this kind of connection can be summarized in the following:

i. The most important establishment is that this (later those) PENROSE—I unit do not reach or connect to the “Central PENROSE—I” biopolymer unit.

ii. It is an opportunity for two kinds of orientation, corresponding to the two basic positions of the PENROSE—I model, as it is illustrated in Plate 5.4., fig. 1,2. In the case of the connection of fig. 1, the surrounding PENROSE-I type skeleton will be heterogeneous taking its surface. In the case of the so-called periodic position the “surface character” will be homogeneous.

iii. The connections of these units with the previous first surrounding skeletons are not uniform. This problem needs further investigations.

iv. Finally such a PENROSE—II model can be assumed too, when the central unit is not completely connected to the surrounding “shell” composed of PENROSE—I units. All these problems together with the problem of the stabilizing biopolymer system will be investigated later.

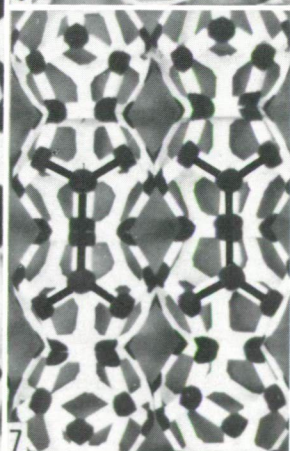
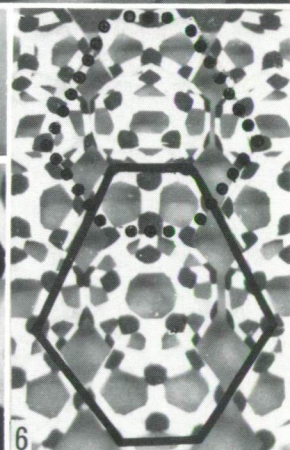
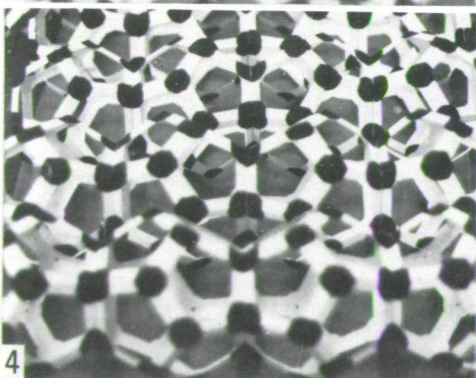
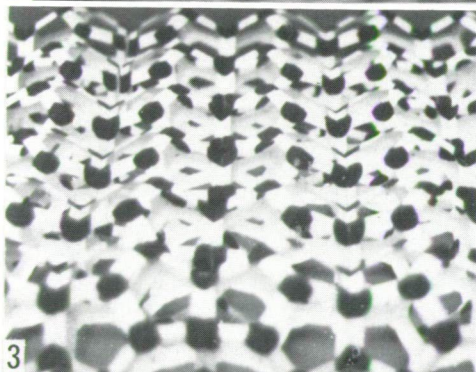
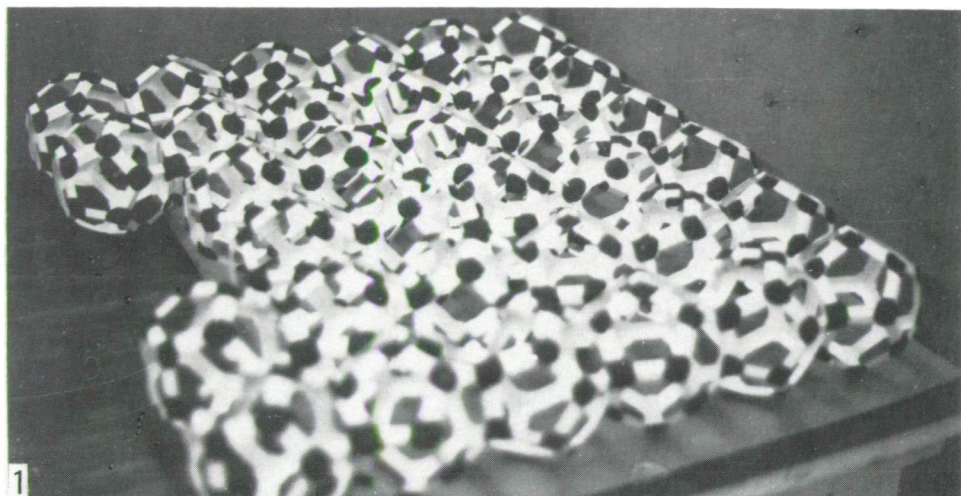
#### Secondary helical biopolymer skeleton (Plate 5.7., figs. 1—7, plate 5.8., figs. 1—4)

As it was emphasized in the previous paper the modelling of the helical biopolymer organization will be continued. In this paper as a new step of the proceeding in this problem the helical model built from PENROSE—I units is presented. To the connections the previously discussed can be said classical, two times three edges method was used. It is necessary to emphasize that during the building of this model it was observed that there are several opportunities for the connections, which can be resulted in helical systems of different deviation diameter. As the final results of several essays, the illustrated model was completed.

#### ◀ Plate 5.9.

- 1—6. Quasi-crystalloid modelling of the primary lamellar biopolymer structures.
1. Front view of the model of the staggered lamella. It is necessary to point out that in this view all kinds of symmetries can be observed. The most important biopolymer symmetry configurations are numbered.
2. Lateral view of one primary lamella. The periodicity in the modelling symmetry is identical with those at the primary filament, cf. Plate 5.1., fig. 3.
3. Above view of the two layered lamella model. Worth of mentioning is a peculiar hexagon.
4. Slightly obliquely lateral view of the quasi-crystalloid skeleton of the two -layered lamella. The connections between the two lamellar systems are important at this kind of modelling.
5. Front view of the model of the staggered lamella, but from different angles in contrast to picture 1 of this Plate.
6. General survey picture from this modelling.





The photographs taken from different views well represent the complexity of the biopolymer system in such a biological primary important biopolymer structure. This helical system results important and interesting periodicity in its basically quasi-periodic units. This periodicity is inside the helical system, without alterations inside the helical line. For a basic PENROSE—I unit the sixth one is in a superponal position. The deviation of this helical model is about 168 Å. Pictures of larger magnification (Plate 5.8., figs. 1—4) well illustrates the points of symmetries of this biopolymer model.

#### Primary lamellar biopolymer structures (Plate 5.9., figs. 1—6)

It is self-understanding that all biological surfaces are extremely important in several points of view. The delimitation inside or outside the biological systems, and its most important characteristic features were the subject of several studies. It is necessary to cite again as fundamentally important establishments the following:

1. The surface of the exine is anionic (ROWLEY, 1971).

2. “the wall itself is a molecular sieve”, p. 449, ROWLEY (1973). After the first discovery of the regular pentagonal polygon biopolymer structure in the pollen exine (KEDVES, 1988), at the first two dimensional scheme for the organization levels of the sporopollenin (KEDVES, 1989, p. 63), the lamellar biological molecular system was also pointed out as an important one.

The three dimensional model was prepared as follows. Two fibrillar units were connected. These so called elementary lamellar model units were prepared by different sizes; the length of 2, 3, 4, 5 and 6 pentagon dodecahedrane units. In this way a staggered lamellar model was completed (Plate 5.9., fig. 6), and investigated by different views. The lateral view of one lamella (Plate 5.9., fig. 2) resulted naturally, the identical periodicity which was established at the primary filament (cf. Plate 5.1., fig. 3). The staggered lamella in front of view of its plane (Plate 5.9., fig. 1 and 6) was investigated by different angles and resulted in interesting and important points of symmetries. In picture no 1 of Plate 5.9. all important systems of symmetry were observed such as rhombus, triangle, hexagon and pentagon. In this way this is another opportunity to explain the results of the non-fivefold rotations, in general the modified MARKHAM rotation method.

From above is photographed a two layered quasi-crystalloid skeleton lamellar model, among the numerous points of symmetry systems and interesting hexagon was pointed out (Plate 5.9., fig. 3). This is in the centrum of the model. The slightly

#### ◀ Plate 5.10.

1—7. Primary modelling of the surface or delimitate quasi-crystalloid layer.

1. General survey aspect of this kind of modelling.

2. Lateral view of this layer.

3, 4. Slightly obliquely lateral view of the surface. These pictures were taken from different angles.

5—7. Points of symmetries of the surface from right angle of the surface plane. The most important configurations are marked.

obliquely lateral view of the two-layered lamella (Plate 5.9., fig. 4) well represents the connections between the two quasi-crystalloid lamellae, different from the above discussed models, cf. Plate 5.9., fig. 1, 5 and 6.

The surface of delimitate quasi-crystalloid layer  
(Plate 5.10., figs. 1–7)

A uni-layered quasi-crystalloid skeleton was investigated. As a general aspect, fig. 1, in Plate 5.10. is presented. The lateral view is identical with the above discussed ones at the filament (Plate 5.1., fig. 3) and at the uni-layered lamella (Plate 5.9., fig. 2). The pictures taken from different angles of the surface resulted in different systems of points of symmetries (Plate 5.10., fig. 3, 4). The perpendicular views are the most interesting and well represent the peculiar characteristic features of this kind of quasi-periodic system. Fig. 5, of Plate 5.10. represents the connections between the two filamental units. The centrum of the middle tetragon is essentially in the right angle of the surface. The previously mentioned hexagonal system (Plate 5.10., fig. 6) and the parallel short axes (Plate 5.10., fig. 7) were pointed out.

### Discussion and conclusions

I hope that with this paper a remarkable proceeding was made to the knowledge of the quasi-crystalloid biopolymer structures. But further investigations in this respect seem to be necessary, as it was emphasized in connection with the PENROSE-II quasi-crystalloid skeleton. But at this moment we need more information about the stabilizing biopolymer system and start its modellization together with the quasi-crystalloid skeleton. This project will be realized in all probability in the not so far future.

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